

Pairing in the Three-Band Hubbard Model of the Cu-O Plane

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By a canonical transformation of the three-band Hubbard model, we introduce an effective Hamiltonian for the propagation of two holes doped into the ground state of the Cu-O plane. When the pair belongs to the 1B_2 or 1A_2 Irreducible Representations of the C_{4v} Group, the bare holes do not interact by the on-site repulsion; the effective interaction between the dressed holes is obtained analytically in terms of renormalized matrix elements, and generalizes earlier findings from cluster calculations. The Fermi liquid is unstable and numerical estimates with reasonable parameters of the binding energy of the pair are in the range of tens of meV. Our scheme naturally lends itself to embody phonon-mediated and other interactions which cannot occur in the Hubbard model but may give important contributions.

The discovery of high- T_C superconductivity [1] has stimulated several serious and ingenious proposals for the pairing mechanism, ranging from enhanced BCS-type [2] and polaron [3] to a variety of purely electronic ones [4–6], just to cite a few of the less exotic proposals. These proposals have usually been regarded as alternative, but there is a clear need for a theoretical framework where they can coexist and can be compared on equal footing, since all the serious mechanisms must convey part of the physics. Our first aim here is to propose such a scheme. Our approach started with cluster calculations in the three-band Hubbard model; pioneers in this field [8,9] explored the possibility that pairing could result from repulsion; later it was pointed out [7] that $W=0$ pairs have intriguing properties. $W=0$ pairs are two-hole eigenstates of the kinetic energy H_0 that are also eigenstates of the on-site repulsion term W with eigenvalue 0. The symmetry of the cluster is an essential ingredient, because only fully symmetric clusters allow such solutions. The planar lattice structure is also essential, because no $W=0$ pairs occur in 3D or in a continuous model. The cluster calculations [10–12] showed that $W=0$ pairs are the "bare" quasiparticles that, when "dressed", become a bound state. That approach is inherently limited by the small size of solvable clusters, but allows a very explicit display of paired hole properties, that even show superconducting flux-quantization [13]. The main indirect interaction through the background particles arises from the second-order contributions to the two-hole amplitude [13]. Our second task here is to extend the theory to the full plane. The three-band Hubbard model Hamiltonian is $H = H_0 + W$, and the independent hole hamiltonian reads, in the site representation

$$H_0 = \sum_{Cu} \varepsilon_d n_d + \sum_O \varepsilon_p n_p + t \sum_{n.n.} [c_p^\dagger c_d + h.c.] \quad (1)$$

where n.n. stands for nearest neighbors. The on-site repulsion Hamiltonian will be denoted by

$$W = \sum_i U_i n_{i+} n_{i-}; \quad (2)$$

where $U_i = U_d$ for a Cu site, $U_i = U_p$ for an Oxygen. Omitting the band indices, we shall mean

$$d[k] = \|k_+, -k_-\| = c_{k_+,+}^\dagger c_{-k,-}^\dagger |vac\rangle \quad (3)$$

to be a two-hole determinantal state derived from the k eigenfunctions.

The point symmetry Group of the Cu-O plane is C_{4v} , and its character Table is shown in Table 1. We introduce the determinants $Rd[k] = d[Rk]$, $R \in C_{4v}$, and the projected states

$$\Phi_\eta[k] = \frac{1}{\sqrt{8}} \sum_{R \in C_{4v}} \chi^{(\eta)}(R) Rd[k] \quad (4)$$

where $\chi^{(\eta)}(R)$ is the character of the operation R in the Irreducible Representation (Irrep) η . In the non-degenerate Irreps, the operations that produce opposite Rk have the same character, and the corresponding projections lead to singlets. Let $R_i, i = 1, \dots, 8$ denote the operations of C_{4v} and k, k' any two points in the Brillouin Zone (BZ). Consider any two-body operator \hat{O} , which is symmetric ($R_i^\dagger \hat{O} R_i = \hat{O}$), and the matrix with elements $O_{i,j} = \langle d[k] | R_i^\dagger \hat{O} R_j | d[k'] \rangle$, where k and k' may be taken to be in the same or in different bands. This matrix is diagonal on the basis of symmetry projected states, with eigenvalues

$$O(\eta, k, k') = \sum_R \chi^{(\eta)}(R) O_R(k, k') \quad (5)$$

where

$$O_R(k, k') = \langle d[k] | \hat{O} | Rd[k'] \rangle. \quad (6)$$

Thus, omitting the k, k' arguments, we get in particular

$$\begin{aligned} O(^1A_2) &= O_E + O_{C_2} + O_{C_4} + O_{C_4^3} \\ &\quad - O_{\sigma_x} - O_{\sigma_y} - O_{\sigma'_1} - O_{\sigma'_2} \end{aligned} \quad (7)$$

$$\begin{aligned} O(^1B_2) &= O_E + O_{C_2} - O_{C_4} - O_{C_4^3} \\ &\quad - O_{\sigma_x} - O_{\sigma_y} + O_{\sigma'_1} + O_{\sigma'_2} \end{aligned} \quad (8)$$

If \hat{O} is identified with W , since $W_E = W_{C_2} = W_{\sigma_x} = W_{\sigma_y}$ and $W_{C_4} = W_{C_4^3} = W_{\sigma'_1} = W_{\sigma'_2}$, one finds $W(^1A_2) = W(^1B_2) = 0$. These are $W=0$ pairs, like those studied previously [13]. One necessary condition for pairing in clusters is that the least bound holes form such a pair, and this dictates conditions on the occupation number. In the full plane, however, $W=0$ pairs exist at the Fermi level for any filling.

Suppose the Cu-O plane is in its ground state with Fermi energy E_F and a couple of extra holes are added.

In principle, by a canonical transformation one can obtain an effective Hamiltonian which describes the propagation of a pair of dressed holes, and includes all many-body effects. Let us see how this arises.

The exact many-body ground state with two added holes may be expanded in terms of excitations over the vacuum (the non-interacting Fermi *sphere*) by a configuration interaction:

$$|\Psi_0\rangle = \sum_m a_m |m\rangle + \sum_\alpha b_\alpha |\alpha\rangle + \sum_\beta c_\beta |\beta\rangle + \dots \quad (9)$$

here m runs over pair states, α over 4-body states (2 holes and 1 e-h pair), β over 6-body ones (2 holes and 2 e-h pairs), and so on. To set up the Schrödinger equation, we consider the effects of the operators on the terms of $|\Psi_0\rangle$. We write:

$$H_0|m\rangle = E_m|m\rangle, H_0|\alpha\rangle = E_\alpha|\alpha\rangle, \dots \quad (10)$$

and since W can create or destroy up to 2 e-h pairs,

$$\begin{aligned} W|m\rangle = & \sum_{m'} V_{m',m} |m'\rangle + \sum_\alpha |\alpha\rangle W_{\alpha,m} \\ & + \sum_\beta |\beta\rangle W_{\beta,m}. \end{aligned} \quad (11)$$

$V_{m',m}$ vanishes for $W=0$ pairs in our model; however we keep it for generality, since it allows to introduce the effect of phonons and any other indirect interaction that we are not considering. For clarity let us first write the equations that include explicitly up to 6-body states; then we have

$$\begin{aligned} W|\alpha\rangle = & \sum_m |m\rangle W_{m,\alpha} + \sum_{\alpha'} |\alpha'\rangle W_{\alpha',\alpha} \\ & + \sum_\beta |\beta\rangle W_{\beta,\alpha} \end{aligned} \quad (12)$$

where scattering between 4-body states is allowed by the second term, and

$$\begin{aligned} W|\beta\rangle = & \sum_{m'} |m'\rangle W_{m',\beta} + \sum_\alpha |\alpha\rangle W_{\alpha,\beta} \\ & + \sum_{\beta'} |\beta'\rangle W_{\beta',\beta} \end{aligned} \quad (13)$$

In principle, the $W_{\beta',\beta}$ term can be eliminated by taking linear combinations of the complete set of β states: when this is done, we get a self-energy correction to E_β and a renormalization of the vertices, without altering the structure of the equations. The Schrödinger equation yields equations for the coefficients a, b and c

$$\begin{aligned} & (E_m - E_0) a_m \\ & + \sum_{m'} a_{m'} V_{m,m'} + \sum_\alpha b_\alpha W_{m,\alpha} + \sum_\beta c_\beta W_{m,\beta} = 0 \end{aligned} \quad (14)$$

$$(E_\alpha - E_0) b_\alpha + \sum_{m'} a_{m'} W_{\alpha, m'} + \sum_{\alpha'} b_{\alpha'} W_{\alpha, \alpha'} + \sum_{\beta} c_\beta W_{\alpha, \beta} = 0 \quad (15)$$

$$(E_\beta - E_0) c_\beta + \sum_{m'} a_{m'} W_{\beta, m'} + \sum_{\alpha'} b_{\alpha'} W_{\beta, \alpha'} = 0 \quad (16)$$

where E_0 is the ground state energy. Then, we exactly decouple the 6-body states by solving the equation for c_β and substituting into the previous equations, getting:

$$(E_m - E_0) a_m + \sum_{m'} a_{m'} \left[V_{m, m'} + \sum_{\beta} \frac{W_{m, \beta} W_{\beta, m'}}{E_0 - E_\beta} \right] + \sum_{\alpha} b_\alpha \left[W_{m, \alpha} + \sum_{\beta} \frac{W_{m, \beta} W_{\beta, \alpha}}{E_0 - E_\beta} \right] = 0 \quad (17)$$

$$(E_\alpha - E_0) b_\alpha + \sum_{m'} a_{m'} W_{\alpha, m'} + \sum_{\alpha'} b_{\alpha'} \left[W_{\alpha, \alpha'} + \sum_{\beta} \frac{W_{\beta, \alpha'} W_{\alpha, \beta}}{E_0 - E_\beta} \right] = 0 \quad (18)$$

Thus we see that the rôle of 6-body states is just to renormalize the interaction between 2-body and 4-body ones, and for the rest they may be forgotten about. If E_0 is outside the continuum of excitations, as we shall show below, the corrections are finite, and experience with clusters suggests that they are small. Had we included 8-body excitations, we could have eliminated them by solving the system for their coefficients and substituting, thus reducing to the above problem with further renormalizations. In principle, the method applies to all the higher order interactions, and we can recast our problem as if only 2 and 4-body states existed. Again, the $W_{\alpha', \alpha}$ term can be eliminated by taking linear combinations of the α states: when this is done, we get a self-energy correction to E_α and a renormalization of the $W_{m, \alpha}$ vertices. The equations become

$$(E_m - E_0) a_m + \sum_{m'} a_{m'} V_{m, m'} + \sum_{\alpha} b_\alpha W_{m, \alpha} = 0 \quad (19)$$

$$(E_\alpha - E_0) b_\alpha + \sum_{m'} a_{m'} W_{\alpha, m'} = 0 \quad (20)$$

Solving for b_α and substituting in the first equation we exactly decouple the 4-body states as well. The eigenvalue problem is now

$$(E_0 - E_m) a_m = \sum_{m'} a_{m'} \{ V_{m, m'} + \langle m | S[E_0] | m' \rangle \}, \quad (21)$$

where

$$\langle m|S[E_0]|m'\rangle = \sum_{\alpha} \frac{\langle m|W|\alpha\rangle\langle\alpha|W|m'\rangle}{E_0 - E_{\alpha}}. \quad (22)$$

This is of the form of a Schrödinger equation with eigenvalue E_0 for pairs with an effective interaction $V+S$. Then we interpret a_m as the wave function of the dressed pair, which is acted upon by an effective hamiltonian \tilde{H} . The change from the full many-body H to \tilde{H} is the canonical transformation we were looking for. However, the scattering operator S is of the form $S = W_{eff} + F$, where W_{eff} is the effective interaction between dressed holes, while F is a forward scattering operator, diagonal in the pair indices m, m' which accounts for the self-energy corrections of the one-body propagators: it is evident from (21) that it just redefines the dispersion law E_m , and, essentially, renormalizes the chemical potential. It is important to realize that therefore F must be dropped. This happens also in the Cooper theory [14], where an effective interaction involving phonons is introduced via an (approximate) canonical transformation; the off-diagonal terms are kept, while the diagonal ones, representing electron self-energy corrections, are dropped. Therefore the effective Schrödinger equation for the pair reads

$$(H_0 + V + W_{eff})|a\rangle = E_0|a\rangle \quad (23)$$

and we are interested in the possibility that $E_0 = 2E_F - \Delta$, with a positive binding energy Δ of the pair. The V interaction just adds to W_{eff} , and this feature allows to include in our model the effects of other pairing mechanisms, like off-site interactions, inter-planar coupling and phonons.

We emphasized the fact that the canonical transformation is exact because in this way our argument does not require U/t to be small. In practice, however, what we can do is to calculate W_{eff} neglecting 6-body and higher excitations, and keeping in mind that at least the structure of the solution is exact when expressed in terms of renormalized matrix elements. So, in the following, we calculate the bare quantities. The α states are 3 hole-1 electron determinants which carry no quasi-momentum. We write

$$|\alpha\rangle = ||(k' + q + k_2)_+, \bar{k}_{2-}, -q_-, -k'_-|| \rangle \quad (24)$$

where \bar{k}_2 is the electron state and pedices refer to the spin direction; those with opposite spin indices contribute similarly and yield a factor of 2 at the end. From the interaction matrix element

$$\begin{aligned} &\langle ||(k' + q + k_2)_+, \bar{k}_{2-}, -q_-, -k'_-|| |W|d[s]\rangle = \\ &\delta(q - s) U(q + k' + k_2, -k', s, k_2) \\ &- \delta(k' - s) U(q + k' + k_2, -q, s, k_2) \end{aligned} \quad (25)$$

we find that the product in the numerator of (22) yields 4 terms; two are proportional to $\delta(p - s)$ and belong to F , while the cross terms yield identical contributions to W_{eff} . Using (5,6), we obtain the effective interaction between $W=0$ pairs:

$$\langle \Phi_\eta[p] | W_{eff} | \Phi_\eta[s] \rangle = 4 \sum_{R \in C_{4v}} \chi^{(\eta)}(R) \sum_{k_2: \varepsilon(Rs+p+k_2) > E_F}^o$$

$$\frac{U(p, k_2, Rs + p + k_2, -Rs) U(Rs + p + k_2, -p, Rs, k_2)}{\varepsilon(Rs + p + k_2) + \varepsilon(s) + \varepsilon(p) - \varepsilon(k_2) - E_0}$$

The sum is over occupied k_2 with empty $Rs + p + k_2$. Note that W_{eff} does not depend on the sign of U . The diagonal elements recover the Δ expression derived from perturbation theory for clusters [13] if E_0 is replaced by the unperturbed eigenvalue $2\varepsilon(p)$.

Since actually $V = 0$ in our model, we drop it in the following. The m and m' indices run over the projected eigenstates $\Phi_\eta[k]$ of the kinetic energy, and the k labels run over $1/8$ of the BZ. We denote such a set of empty states $e/8$, and cast the result in the form of a (Cooper-like) Schrödinger equation

$$2\varepsilon(k) a(k) + \sum_{k'}^{e/8} W_{eff}(k, k') a(k') = E_0 a(k) \quad (26)$$

for a self-consistent calculation of E_0 (since W_{eff} depends on the solution). Let N_C be the number of cells in the crystal. The U matrix elements scale as N_C^{-1} and therefore W_{eff} scales in the same way. For an infinite system, $N_C \rightarrow \infty$, this is a well defined, but quite intractable integral equation. The problem becomes discrete when working with a supercell of $N_{SC} \times N_{SC} = N_C$ cells, with periodic boundary conditions. However, Δ depends on U 's and N_C in a complicated way, within the range of attainable supercell sizes. We define the Uniform Interaction Model (UIM) in which a constant effective interaction V prevails for k and k' in $1/8$ of the empty part of the BZ. Having computed Δ for a given filling and N_{SC} according to (26) we can determine the value of V which gives the same Δ in the UIM. This will be V_{eff} , that is, the effective V of our theory, characterizing the strength of the attraction by a single quantity. Since V_{eff} is not strongly size dependent, its numerical convergence with increasing N_{SC} is observed. In addition, the UIM can be solved in the thermodynamic limit; writing $E_0 = 2E_F - \Delta$ we can estimate Δ_{asympt} for $N_C \rightarrow \infty$. Indeed, the Cooper-like Schrödinger equation (26) with $W_{eff} = -\frac{V}{N_C}$, $V > 0$, leads to

$$\frac{8}{V} = \int_{E_F}^0 \frac{d\varepsilon \rho(\varepsilon)}{2(\varepsilon - E_F) + \Delta_{asympt}} \quad (27)$$

where ρ is the density of states, which is solved numerically. We use as input data the current estimates (in eV) $t=1.3$, $\varepsilon_p=3.5$, $\varepsilon_d=0$, $U_p=6s$, $U_d=5.3s$, where s is a scale factor induced by renormalization.

At $s=2.121$, with $E_F=-1.3$ eV, we get for 1B_2 pairs the results shown in Table II. Here, n_{tot} is the filling and V_{eff} is derived by comparison with UIM calculations. We see that V_{eff} is fairly stable when increasing

the supercell size and corresponds to Δ_{asymp} values of about 20 meV. Convergence to the thermodynamic limit is achieved, and implies a Cooper-like instability of the Fermi liquid in this model of the Cu-O plane. Δ_{asymp} values in the range of several tens to a few hundreds of meV are obtained with a scale s which is somewhat larger than 1; it could be that the current estimates of U 's are a bit low; however, since the screening excitations are explicitly accounted for in the Hamiltonian, it is reasonable that the input U 's must be somewhat larger than the fully screened interaction. Moreover, contributions from phonons and other mechanisms can be included by a non zero V , and must be relevant for a comparison with experiment. We find that 1A_2 pairs are more tightly bound close to half filling, but 1B_2 pairs are favored when the filling increases. We get attraction and pairing at all fillings: since the present mechanism is driven by symmetry it works unless the system distorts. Further data will be presented elsewhere.

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Tables

C_{4v}	E	C_2	$2C_4$	2σ	$2\sigma'$	
A ₁	1	1	1	1	1	
A ₂	1	1	1	-1	-1	R_z
B ₁	1	1	-1	1	-1	$x^2 - y^2$
B ₂	1	1	-1	-1	1	xy
E	2	-2	0	0	0	(x, y)

TABLE I. The Character Table of the C_{4v} Group

N_{SC}	n_{tot}	$\Delta (meV)$	$V_{eff} (eV)$	$\Delta_{asympt} (meV)$
18	1.13	121.9	7.8	41.6
20	1.16	42.2	5.	9.0
24	1.14	59.7	7.	28.9
30	1.14	56.	5.7	13.2
40	1.16	30.5	6.6	23.4

TABLE II. Binding Energy of W=0 Pairs.